K_2NiF_4 Structure: A4B2C_tI14_139_ce_e_a-001

This structure originally had the label `A4B2C_tI14_139_ce_e_a`. Calls to that address will be redirected here.

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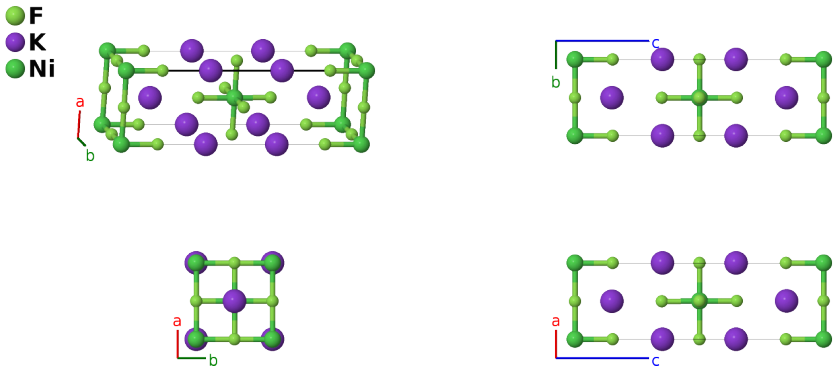
https://aflow.org/p/SENW

https://aflow.org/p/A4B2C_tI14_139_ce_e_a-001



Prototype	F_4K_2Ni
AFLOW prototype label	A4B2C_tI14_139_ce_e_a-001
ICSD	15576
Pearson symbol	tI14
Space group number	139
Space group symbol	$I4/mmm$
AFLOW prototype command	`aflow --proto=A4B2C_tI14_139_ce_e_a-001 --params=`$a, c/a, z_3, z_4$

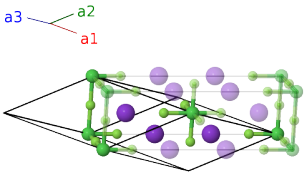
Other compounds with this structure

Ba_2SnO_4, Ca_2MnO_4, Cs_2CrCl_4, Cs_2CrF_4, Cs_2CuCl_4, Cs_2CuF_4, K_2CrCl_4, K_2CrF_4, K_2CuCl_4, K_2CuF_4, La_2NiO_4, La_2PdO_4, Nd_2CuO_4, Sr_2IrO_4, Sr_2MnO_4, Sr_2RuO_4, Sr_2SnO_4, Sr_2TiO_4, Sr_2VO_4, $(Fe, La)_2SrO_4$, $(Sr, La)_2AlO_4$, $(Sr, La)_2CoO_4$

- This is the parent compound of the simplest layered-perovskite Ruddlesden-Popper series (Wikipedia). The series also includes the parent of the high-T_c cuprates, $(La,Ba)_2CuO_4$, but we keep that separate as it represents a new class of materials.
- $Sr_2CuO_2Cl_2$ is the quaternary form of this structure.

Body-centered Tetragonal primitive vectors

$$\mathbf{a_1} = -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} - \tfrac{1}{2}c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Ni I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}}$	(4c)	F I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(4c)	F I
$\mathbf{B_4}$	=	$z_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_2$	=	$cz_3\,\hat{\mathbf{z}}$	(4e)	F II
$\mathbf{B_5}$	=	$-z_3\,\mathbf{a}_1 - z_3\,\mathbf{a}_2$	=	$-cz_3\,\hat{\mathbf{z}}$	(4e)	F II
$\mathbf{B_6}$	=	$z_4\,\mathbf{a}_1 + z_4\,\mathbf{a}_2$	=	$cz_4\,\hat{\mathbf{z}}$	(4e)	K I
$\mathbf{B_7}$	=	$-z_4\,\mathbf{a}_1 - z_4\,\mathbf{a}_2$	=	$-cz_4\,\hat{\mathbf{z}}$	(4e)	K I

References

[1] D. Balz and K. Pleith, *Die Struktur des Kaliumnickelfluorids, K_2NiF_4*, Z. Elektrochemie **59**, 545–551 (1955).

Found in

[1] S. N. Ruddlesden and P. Popper, *New compounds of the K_2NiF_4 type*, Acta Cryst. **10**, 538–539 (1957), doi:10.1107/S0365110X57001929.